

Naval Environmental Prediction Research Facility

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TESTS OF VARIOUS FINITE DIFFERENCE
ALGORITHMS APPLIED TO A SIMPLE
WATER VAPOR TRANSPORT PROBLEM
ON A STAGGERED GRID

Hung-Chi Kuo

Naval Environmental Prediction Research Facility

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1. INTRODUCTION

With the advent of large digital computers, numerical modeling has taken an important place in atmospheric science. Constructing a numerical model often involves two steps. The first step is to formulate a set of continuous equations which represent the dynamics and the physics of interest in the atmosphere. The second step is to discretize these equations so that they may be solved on a computer.

Broadly speaking, the discretization methods for solving the continuous equations may be grouped as Eulerian or Lagrangian (fully Lagrangian or semi-Lagrangian) methods. The Eulerian methods may be further classified according to the techniques employed for the integration in time and the approximations used for the spatial derivatives. The integration in time can be either explicit or implicit (fully implicit or semi-implicit) while the spatial discretization may themselves be grouped under two general headings: series expansion methods and finite difference methods. The Galerkin procedure is often involved in the series expansion methods. Some commonly used series expansion methods are finite element, spectral and collocation. In the finite difference method, the flux form is often preferred to the advective form in order to maintain in the discretized equations integral constraints of the continuous atmosphere. In addition, the variables are staggered around the grid points for the sake of better geostrophic adjustment. Of the staggered grids B, C, D and E (Arakawa and Lamb, 1977), the C-grid has found favor amongst numerical modelers (Arakawa and Lamb, 1977; Schoenstadt, 1978) despite criticisms raised by some authors

(Mesinger, 1973). There are very few finite difference models that employ a non-staggered grid. The C-grid is currently used in the Navy Operational Regional Atmospheric Prediction System (Hodur, 1982, 1987).

There are many problems in environmental science where a central concern is the manner in which a trace constituent or water vapor is transported by moving fluid. It is important to find a suitable finite difference algorithm on a staggered grid for this problem. In this report, we use a simple water vapor transport problem (i.e., one-dimensional linear advection of water vapor) to study the advective processes on the staggered grid. It is illustrated that caution must be taken in defining flux on the staggered C-grid. It is shown that accuracy can be lost in the fourth-order centered differencing if flux is defined improperly. A consistent way of defining flux with the fourth-order finite differencing is presented.

2. MODEL PROBLEM AND DISCRETIZATION SCHEMES

To illustrate the points mentioned above, we use finite difference schemes to discretize the one-dimensional, constant coefficient ($u = \text{const.}$) advection equation

$$\frac{\partial q}{\partial t} + u \frac{\partial q}{\partial x} = 0 \quad (2.1)$$

in the periodic domain $[-1,1]$ with the initial condition

$$q(x, t = 0) = \exp \left[- \left(\frac{x}{0.2} \right)^2 \right]. \quad (2.2)$$

This problem is the simplest prototype of a model involving wave or advective processes. For the test purpose, Eq. (2.1) can be easily written in flux form as

$$\frac{\partial q}{\partial t} + \frac{\partial F}{\partial x} = 0 \quad (2.3a)$$

$$F = uq \quad (2.3b)$$

and solved on the staggered grid shown in Figure 1. Note that the flux is defined on the velocity point. Since the q points and flux points are staggered, we shall define the flux in terms of surrounding q values and consider the spatial derivative by either second-order or fourth-order centered differences. Schemes (I)-(V), which involve different ways to define the flux and to approximate the spatial derivative, are used to discretize (2.3). The definition of flux and space differencing of these schemes are as follows:

Scheme (I)

$$\frac{\partial q_i}{\partial t} = - \delta_x F_i \quad (2.4a)$$

$$F_{i+1/2} = \frac{(u_{i+1/2} + |u_{i+1/2}|)}{2.0} q_i + \frac{(u_{i+1/2} - |u_{i+1/2}|)}{2.0} q_{i+1}. \quad (2.4b)$$

Scheme (II)

$$\frac{\partial q_i}{\partial t} = - \left(\frac{9}{8} \delta_x F_i - \frac{1}{8} \delta_{3x} F_i \right) \quad (2.5a)$$

$$F_{i+1/2} = \frac{(u_{i+1/2} + |u_{i+1/2}|)}{2.0} q_i + \frac{(u_{i+1/2} - |u_{i+1/2}|)}{2.0} q_{i+1}. \quad (2.5b)$$

Scheme (III)

$$\frac{\partial q_i}{\partial t} = - \delta_x F_i \quad (2.6a)$$

$$F_{i+1/2} = \frac{q_i + q_{i+1}}{2.0} u_{i+1/2} \quad (2.6b)$$

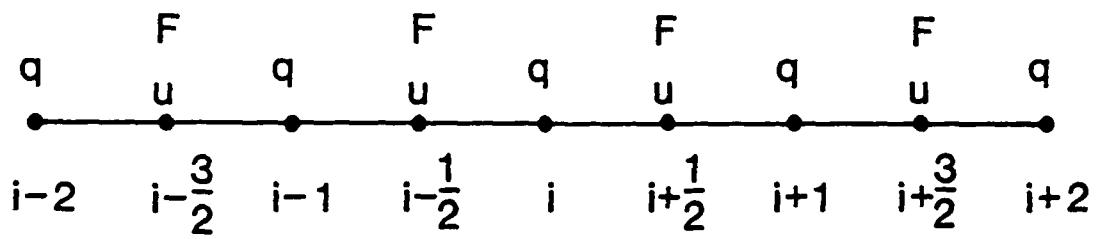


Figure 1. Staggered grid of two variables.

Scheme (IV)

$$\frac{\partial q_i}{\partial t} = - \left(\frac{9}{8} \delta_x F_i - \frac{1}{8} \delta_{3x} F_i \right) \quad (2.7a)$$

$$F_{i+1/2} = \frac{q_i + q_{i+1}}{2.0} u_{i+1/2} \quad (2.7b)$$

Scheme (V)

$$\frac{\partial q_i}{\partial t} = - \left(\frac{9}{8} \delta_x F_i - \frac{1}{8} \delta_{3x} F_i \right) \quad (2.8a)$$

$$F_{i+1/2} = [9/16(q_{i+1} + q_i) - 1/16(q_{i+2} + q_{i-1})] u_{i+1/2} \quad (2.8b)$$

where

$$\delta_x F_i = \frac{F_{i+1/2} - F_{i-1/2}}{\Delta x} \text{ and } \delta_{3x} F_i = \frac{F_{i+3/2} - F_{i-3/2}}{3\Delta x}$$

Forward time integration is used in Scheme (I) and (II) while the second-order leapfrog time integration is used in Schemes (III), (IV) and (V) for their time discretization. To suppress the computational mode in the leapfrog time integration, an Asselin filter with a damping coefficient of 0.02 is used. Note that the first-order upstream flux is used in both Schemes (I) and (II), while the second-order flux is used in Schemes (III) and (IV). The flux in Scheme (V) is fourth-order in accuracy according to the Taylor expansion. The spatial derivatives are approximated by either second-order centered differencing (Schemes (I) and (III)) or fourth-order centered differencing (Schemes (II), (IV) and (V)). Thus, Schemes (III)

and (V) define the flux and approximate the spatial derivative with the same order of accuracy (i.e., second-order for (III) and fourth-order for (V)). In the linear advection equation, space differencing of Scheme (I) is the same as the first-order upstream differencing. Note that Schemes (II) and (IV) involve a mixture of accuracy in defining flux and approximating the spatial derivatives. The fourth-order Scheme (V), which is for the C-grid even in a two-dimensional situation, is analogous to the scheme described by Gerrity et al. (1972) for the non-staggered grid and Campana's (1973) implementation for the B-grid.

Recently, Professor A. Arakawa (personal communication), in the context of solving the continuity equation in a primitive equation model using isentropic surfaces as a vertical coordinate, has proposed a generalization of Takacs' (1985) scheme which has very small computational dispersion and which guarantees positive results. Arakawa's scheme is third-order in accuracy. We will include Arakawa's scheme in our results for comparison. Formulation of Arakawa's scheme is presented in Appendix A. In addition to Arakawa's method, we will also test the positive definite advection scheme of Smolarkiwicz (1983). Similar to Arakawa's method, Smolarkiwicz's method involves predictor-corrector procedure; but, the cost of Smolarkiwicz's method is lower compared to Arakawa's method. Detail of Smolarkiwicz's scheme is in Appendix B.

3. MODEL PROBLEM ANALYSIS

For the one-dimensional constant coefficient advection equation, Scheme (I) employs the first-order upstream differencing while Scheme (III) employs the second-order centered differencing. Detailed analysis of Scheme (I) and Scheme (III) for the one-dimensional linear advection equation can be found in Haltiner and Williams (1980). To better understand the accuracy and stability properties of Schemes (IV) and (V) we now follows an argument similar to that given by Haltiner and Williams (1980). Consider the following fourth-order, space-centered differencing and leapfrog time differencing for the constant coefficient advection (Eq. (2.1)).

$$\frac{q_m^{n+1} - q_m^{n-1}}{2\Delta t} = -u(a \frac{q_{m+1}^n - q_{m-1}^n}{2\Delta x} + b \frac{q_{m+2}^n - q_{m-2}^n}{4\Delta x} + c \frac{q_{m+3}^n - q_{m-3}^n}{6\Delta x}). \quad (3.1)$$

Since each of the terms with coefficients a , b and c are valid approximations for $\partial F/\partial x$, it is clear that (3.1) will be a consistent scheme provided that $a + b + c = 1$. The requirement for (3.1) to be fourth-order accurate is that the second-order truncation terms vanish. This implies that the sum of the Taylor series terms

$$a(\frac{\partial^3 q}{\partial x^3}) \Delta x^3 / 3!(2\Delta x), \quad b(\frac{\partial^3 q}{\partial x^3}) (2\Delta x)^3 / 3!(4\Delta x),$$

and a similar term,

$$c(\frac{\partial^3 q}{\partial x^3}) (3\Delta x)^3 / 3!(6\Delta x),$$

from series expansions for $q_{m\pm 1}^n$, $q_{m\pm 2}^n$ and $q_{m\pm 3}^n$ must vanish. Thus the resulting truncation error in (3.1) is $O(\Delta t^2) + O(\Delta x^4)$ if

$$a + 4b + 9c = 0. \quad (3.2)$$

The stability will be investigated next. Using the usual notation, we assume a solution of the form

$$q_m^n = A e^{i\alpha n \Delta t} + i\mu m \Delta x \quad (3.3)$$

and define

$$f(\mu \Delta x) = a \sin \mu \Delta x + \frac{b}{2} \sin 2 \mu \Delta x + \frac{c}{3} \sin 3 \mu \Delta x \quad (3.4)$$

$$f'(\mu \Delta x) = a \cos \mu \Delta x + b \cos 2 \mu \Delta x + c \cos 3 \mu \Delta x. \quad (3.5)$$

Substitution of (3.3) into (3.1) leads to

$$\sin \alpha \Delta t = - \frac{u \Delta t}{\Delta x} f(\mu \Delta x). \quad (3.6)$$

If α is real, neutral solutions result with no damping or amplification, as evident from (3.3). The condition for a real is that the right side of (3.6) has magnitude less than or equal to 1, otherwise it is complex. To insure stability for all wavelengths, it is necessary to find the maximum magnitude of $f(\mu \Delta x)$. Let $f[(\mu \Delta x)_{\max}]$ be the maximum value of $f(\mu \Delta x)$. Then the following criterion must be satisfied to maintain stability for all wave numbers.

$$\left| \frac{u \Delta t}{\Delta x} \right| \leq 1 / |f[(\mu \Delta x)_{\max}]|. \quad (3.7)$$

The phase speed and group velocity resulting from the discretization of (3.1) can also be derived. The phase velocity C_p is

$$C_p = u * \frac{1}{\mu \Delta x \ CR} \sin^{-1} [CR * f(\mu \Delta x)] \quad (3.8)$$

while the group velocity C_g is

$$C_g = u * f'(\mu \Delta x) / (1 - [CR * f(\mu \Delta x)])^{1/2} \quad (3.9)$$

where CR is the Courant number.

For the one-dimension linear advection problem, we can easily rearrange the leapfrog time discretization of (2.7) and (2.8) into the form of (3.1). We will get $a = 13/12$, $b = -1/12$ and $c = 0$ for Scheme (IV) and $a = 87/64$, $b = -3/8$ and $c = 1/64$ for Scheme (V). Note that for the non-staggered grid with fourth-order difference, as given in Haltiner and Williams (1980), $a = 4/3$, $b = -1/3$ and $c = 0$. Although Schemes (IV) and (V) are consistent, Scheme (IV) is not a fourth-order scheme because it violates (3.2). Note that the minimum resolvable wavelength of $2\Delta x$ is stationary in both Schemes (IV) and (V) according to (3.8). Also there are physical and computational modes in the numerical solutions as revealed by (3.8).

The group velocity for a $2\Delta x$ length in Scheme (V) is strongly negative with $C_g = -7/4u$ while the group velocity for a $4\Delta x$ length with $CR = 0.7$ is almost the same as u . It can be concluded therefore that Scheme (V) can lead to more rapid spreading of noise to the phase velocity in the very short wavelengths from any source in the model, physical or computational. Table 1 gives the ratio of finite difference wave speed

Table 1. C_F/u as functions of CR and Δx .

Schemes	CR	$2\Delta x$	$4\Delta x$	$6\Delta x$	$8\Delta x$	$10\Delta x$	$12\Delta x$
Non-staggered 4th Order							
(IV)							
$a = 4/3$	0.2	0	0.86	0.97	0.99	1.00	1.00
$b = -1/4$	0.4	0	0.89	0.99	1.00	1.01	1.01
$c = 0$	0.6	0	0.98	1.03	1.03	1.02	1.01
(V)							
$a = 87/64$	0.2	0	0.87	0.97	0.99	0.99	0.99
$b = -3/8$	0.4	0	0.91	0.99	1.00	1.00	1.00
$c = 1/64$	0.6	0	1.00	1.04	1.03	1.01	1.01

to true wave speed, C_F/u , as a function of wavelength in terms of Δx versus Courant number CR for Schemes (IV), (V) and the non-staggered fourth-order finite difference for the constant coefficient advection equation. From Table 1, we conclude that Scheme (IV) is only of second-order accuracy despite the additional calculation performed for the fourth-order spatial derivative and Scheme (V) is a proper implementation of the fourth-order finite difference scheme on the staggered grid shown in Figure 1.

In view of the significant accuracy improvement in the fourth-order schemes, as compared to the second-order schemes, we now concentrate on the stability analysis of the fourth-order

Scheme (V). With the parameters a , b and c in Scheme (V), we found that $(u\Delta x)_{\max} \approx 75^\circ$ and the stability condition (3.7) of Scheme (V) gives

$$|ICR| = \left| \frac{u\Delta t}{\Delta x} \right| \leq 0.71 . \quad (3.10)$$

Equation (3.10) indicates that the CFL criterion associated with Scheme (V) is more restrictive, and, for a given u and Δx , the time step would have to be 29 percent smaller for the fourth-order Scheme (V) versus the second-order Scheme (III). Note that the CFL criterion of Scheme (V) is the same as the non-staggered fourth-order finite difference of Haltiner and Williams (1980)

4. NUMERICAL RESULTS

A very small time step is used in the time integrations presented in this section so that the error in the computation is dominated by the spatial discretization error due to finite difference methods.

Figure 2 shows the approximate solutions at $t = 2.0$ obtained by Schemes (I) - (V) and the scheme of Arakawa with number of grid points $N = 32$. Note that Schemes (I) and (II) produces practically identical results when compared with Schemes (III) and (IV). It is clear from Figure 2 that Scheme (V) gives a much better solution than do Schemes (III) and (IV). Schemes (I), (II), and the Smolarkiwicz scheme and Arakawa scheme generates positive definite fields. The Arakawa scheme is associated with the least damping among all the positive-definite schemes.

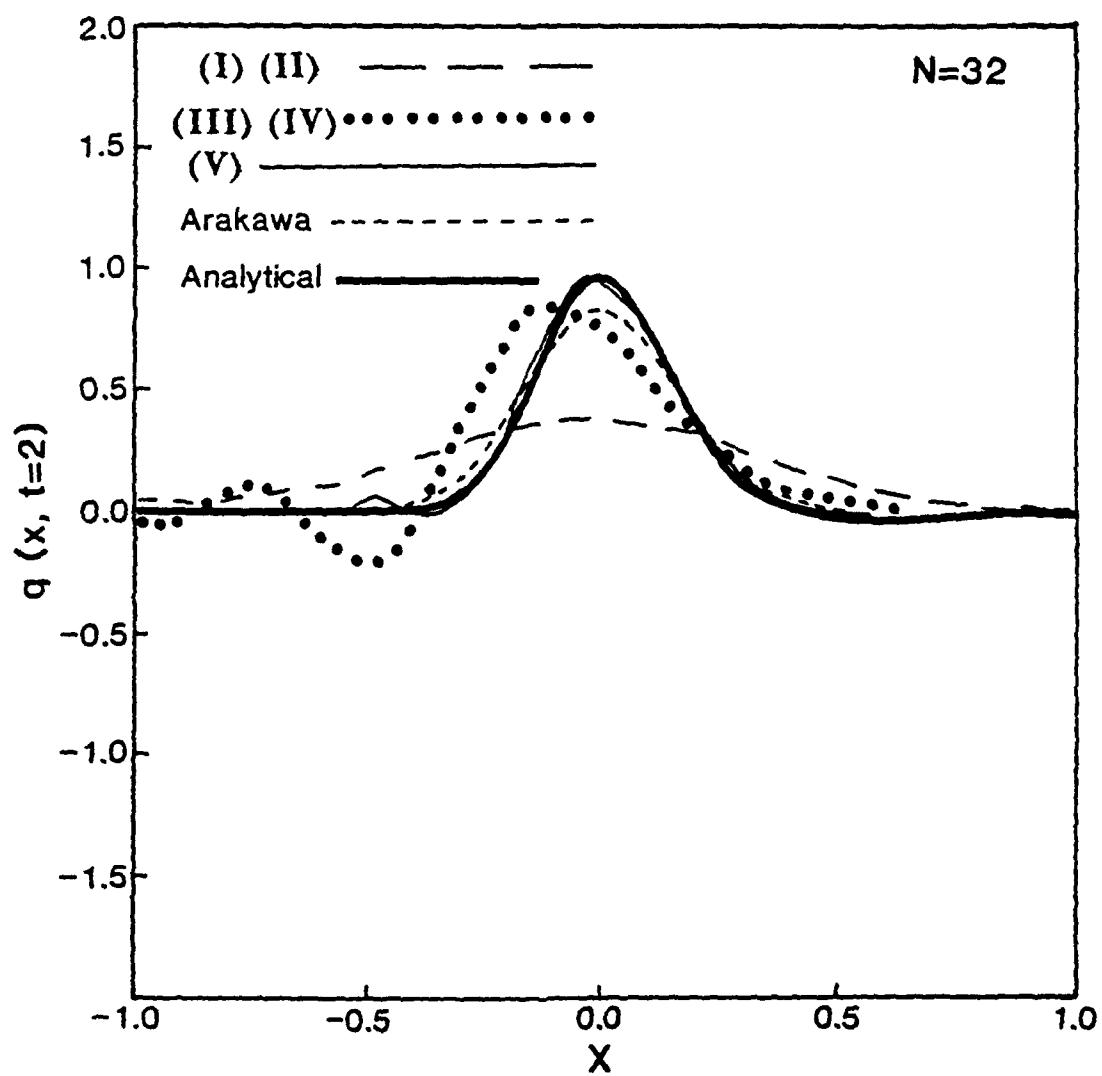


Figure 2. Analytical and numerical solutions with $N=32$ at $t=2$.

Figure 3 illustrates the numerical solutions at $t = 2.0$ obtained by all the positive-definitive schemes. Smolarkiwicz's scheme is tested with various S factors and with two corrective steps. There seems to be a slightly upwind phase shift with the Smolarkiwicz scheme for $S = 1$. Moreover, the choice of S factor does not seem to be straightforward. Both the Arakawa and Smolarkiwicz schemes preserve the mass very well.

Figure 4 shows the corresponding L2 error as a function of the number of grid points for $t = 2.0$.

$$\text{Here L2 error} = \left\{ \frac{1}{N} \sum_{j=1}^N [u(x_j, t) - u_a(x_j, t)]^2 \right\}^{1/2}$$

with $u_a(x_j, t)$ is the analytical solution and $u(x_j, t)$ is a computed solution at grid x_j at time t . The different convergence properties of different schemes can be easily seen from Figure 4. For example, Scheme (I) and (II) converge to the analytical solution with first-order accuracy (as expected from upstream differencing) while Schemes (III) and (IV) converge to the analytical solution with the same second-order accuracy. The fourth-order accuracy of Scheme (V) is obvious when compared to Arakawa's third-order scheme. Figure 3 reinforces the observation from Figure 2 that higher accuracy is associated with the Scheme (V) solution. In particular, the Scheme (V) solution is about ten times more accurate than the Scheme (III) and (IV) solutions with the same number of grid points. Because Scheme (V) only requires less than three times as much computation as Scheme (III), there is a net gain in accuracy by using fourth-order Scheme (V).

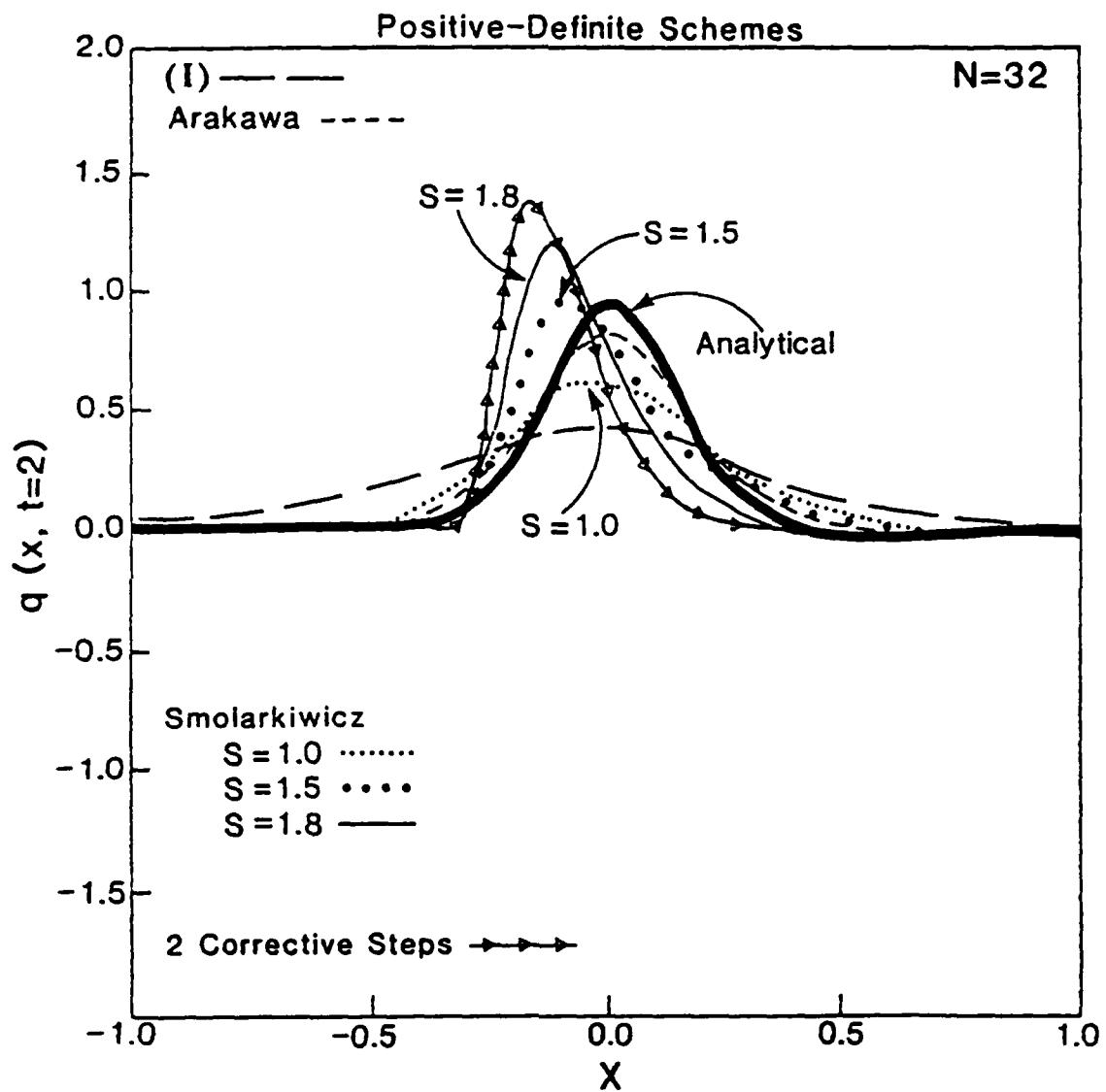


Figure 3. Analytical and numerical solutions of positive definite schemes with $N=32$ at $t=2$.

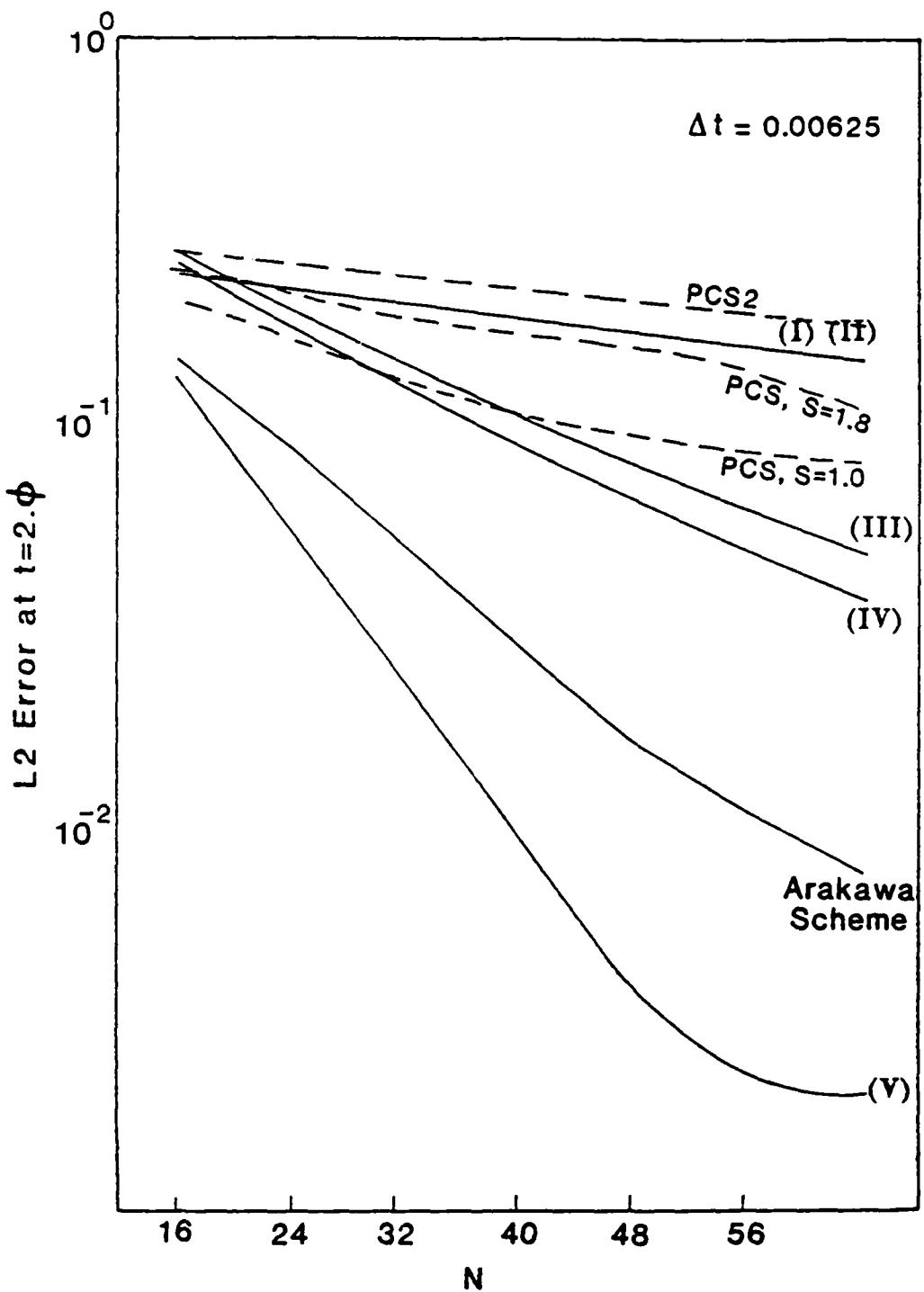


Figure 4. L_2 error in the numerical solutions of the test problem as functions of N (number of grids) at $t=2$.
 PCS is the Smolarkiwicz scheme. PCS2 is the Smolarkiwicz scheme with two corrective steps.

5. CONCLUDING REMARKS

In this report, we used the one-dimensional constant advection of a Gaussian function to test four positive-definite schemes ((I), (II), Smolarkiwicz scheme, and Arakawa scheme) and three even-order accurate schemes ((III), (IV) and (V)) on the staggered grid. It is shown that for the test problem, Schemes (I) and (II) produce identical numerical results. The Arakawa scheme produces the least damping among all the positive-definite schemes; however, there are expensive computations required with the Arakawa scheme. The Smolarkiwicz scheme seems to be cost effective. The slightly upstream shifted phase in numerical solution as well as the determination of the S factor may be the drawback of the scheme. Of the even-order accurate schemes, Scheme (V) produces very accurate results. Stability analysis indicates that a reduction in time step size (29% smaller) is required when Scheme (V) is used instead of Scheme (III). Scheme (V), however, produces results ten times more accurate than Schemes (III) and (IV) with the same number of grid points. Also, Scheme (V) only requires less than three times as much computation as Scheme (III).

Based on the calculations in this report, we suggest that Schemes (II) and (IV) should never be used in a staggered grid model. This is because the accuracy associated with the flux is inconsistent with the accuracy of the approximations to the spatial derivatives. The additional calculations performed in the fourth-order centered differencing in these two schemes do not increase model accuracy.

Finally we recommend that for the purpose of horizontal advection of water vapor mixing ratio on the C-grid, Scheme (V) should replace (IV) in the Navy Operational Regional Atmospheric Prediction System (Hodur 1982, 1987). Improvement of the model accuracy from the replacement is expected.

In closing we note that there are many other algorithms that can be applied to the transport of trace constituent or water vapor in atmospherical models. A more complete review can be found in Rood (1987). In addition to many useful finite difference schemes, there are Lagrangian and series expansion Eulerian methods. The pseudospectral (collocation) and the semi-Lagrangian methods are of special interest. Rasch and Williamson (1989) used shape preserving interpolation schemes in the semi-Lagrangian method to maintain the local monotonicity of the simulated fields. Since the semi-Lagrangian method can be used in conjunction with the finite difference - finite element and spectral approaches with a larger time step than the Eulerian methods - the shape-preserving semi-Lagrangian scheme seems to be very useful.

The efficiency of the spectral or collocation method often lies in its exponential convergence property (Fulton and Schubert, 1987). For the linear advection equation, the pseudospectral method is the same as the Galerkin or tau method except that the $2\Delta x$ wave is stationary in the pseudospectral method. Finite differences on non-staggered grids and Chebyshev collocation methods have been applied to the same advection problem studied in this report (Fulton and Schubert (1987)).

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APPENDIX A

Arakawa's method is in the prediction-correction form.

Predictor:

$$q_i^* = q_i^n - \Delta t \delta_x F_i \quad (A1)$$

where

$$F_{i+1/2} = u_{i+1/2}^+ q_i^n + u_{i+1/2}^- q_{i+1}^n \quad (A2)$$

$$u_{i+1/2}^+ = 0.5 (u_{i+1/2} + |u_{i+1/2}|) \quad (A3)$$

$$u_{i+1/2}^- = 0.5 (u_{i+1/2} - |u_{i+1/2}|) \quad (A4)$$

Corrector:

$$q_i^{n+1} = q_i^n - \Delta t \delta_x F_i^* \quad (A5)$$

where

$$F_{i+1/2}^* = u_{i+1/2}^+ \frac{q_{i+1}^* + q_i^n}{2.0} + u_{i+1/2}^- \frac{q_i^* + q_{i+1}^n}{2.0} + G_{i+1/2} \quad (A6)$$

$$G_{i+1/2} = - \alpha_{i+1/2} [u_{i+1/2}^+ \hat{\rho}_{i+1/2}^+ (q_{i+1}^* - q_i^n) - \\ \hat{u}_{i+1/2}^+ \hat{\rho}_{i+1/2}^+ (q_i^* - q_{i-1}^n)] \quad (A7)$$

$$+ u_{i+1/2}^- \hat{\rho}_{i+1/2}^- (q_i^* - q_{i+1}^n) - \\ \hat{u}_{i+1/2}^- \hat{\rho}_{i+1/2}^- (q_{i+1}^* - q_{i+2}^n)]$$

$$\alpha_{i+1/2} = \frac{1 + |u_{i+1/2}| \frac{\Delta t}{\Delta x}}{6.0} \quad (A8)$$

$$r_{i+1/2}^+ = \frac{1 - 2\alpha_{i+1/2}}{2\alpha_{i+1/2}} r_{i+1/2}^+ + 1 \quad (A9)$$

$$\hat{r}_{i+1/2}^{\pm} = 1 - r_{i+1/2}^{\pm} \quad (A10)$$

$$r_{i+1/2}^+ = \frac{(q_{i-1}^n - 2q_i^n + q_{i+1}^n)^2}{(q_{i-1}^n - 2q_i^n + q_{i+1}^n)^2 + q_i^n q_{i+1}^n + \epsilon} \quad (A11)$$

$$r_{i+1/2}^- = \frac{(q_i^n - 2q_{i+1}^n + q_{i+2}^n)^2}{(q_i^n - 2q_{i+1}^n + q_{i+2}^n)^2 + q_i^n q_{i+1}^n + \epsilon} \quad (A12)$$

$$\hat{u}_{i+1/2}^+ = (u_{i+1/2}^+ u_{i-1/2}^-)^{1/2} \quad (A13)$$

$$\hat{u}_{i+1/2}^- = (|u_{i+1/2}^-| |u_{i+3/2}^-|)^{1/2} \quad (A14)$$

Here the superscript n indicates the nth time level during time integration and $\epsilon = 10^{-15}$.

APPENDIX B

The Smolarkiwicz scheme is in the predictor-corrector form.

Predictor:

$$F_{i+1/2} = \frac{(u_{i+1/2} + |u_{i+1/2}|)}{2.0} q_i^n + \frac{(u_{i+1/2} - |u_{i+1/2}|)}{2.0} q_{i+1}^n \quad (B1)$$

$$q_i^* = q_i^n - \Delta t \delta_x F_i \quad (B2)$$

Corrector:

$$\tilde{u}_{i+1/2} = \frac{(|u_{i+1/2}| \frac{\Delta x}{2.0} - \Delta t u_{i+1/2}^2) (q_{i+1}^* - q_i^*)}{\frac{\Delta x}{2.0} (q_i^* + q_{i+1}^* + \epsilon)} * s \quad (B3)$$

(B4)

$$F_{i+1/2}^* = \frac{(\tilde{u}_{i+1/2} + |\tilde{u}_{i+1/2}|)}{2.0} q_i^* + \frac{(\tilde{u}_{i+1/2} - |\tilde{u}_{i+1/2}|)}{2.0} q_{i+1}^* \quad (B4)$$

$$q_i^{n+1} = q_i^n - \Delta t \delta_x F_i^* \quad (B5)$$

Here $\epsilon = 10^{-15}$, s is an engineer factor used to improve the quality of solution from experiment. The superscript n indicates the nth time level during time integration. The corrector step can be repeated to improve the solution according to Smolarkiwicz (1983). We have also tested the scheme with two corrective steps.

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